

7. FAIR PRINCIPLES AND LINKED DATA: PUBLICATION OF OPEN NOTEBOOK SCIENCE

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7.1 INTRODUCTION

The way to conduct and communicate scientific research has been going through changes. Such changes are caused by advances in technology, overproduction of data, funding pressures and collaborative culture among researchers.

This new way of conducting science contemplates the dissemination of primary data, preferably, as far as they are generated, and not only in successful cases or cases with consolidated results. The tendency is to allow the open simultaneous collaboration to a broad contribution with the purpose of achieving new results.

Notebooks of science are data annotation instruments, generally experimental, produced in laboratory to base scientific publications that are normally published in its final configurations. For Schnell (2015) notebook science reports hypothesis, experiments and initial analysis or interpretations of the experiments, and it works as a legal record of properties of ideas and results obtained by a scientist. It is observed that despite the importance given to data recorded in journals, in its majority it is not published in a structured way so it is reused by human users and machines.

In this context, Web Semantic and FAIR principles stand out to guide the structuring of open notebook science in a way to make it findable, accessible, interoperable and reusable, besides improving the capacity of machines to automatically find and use data and support its reuse by individuals. Therefore, this group presents semantic elements for publishing open notebooks from the application of FAIR principles, in the Web Semantic and *Linked Data* perspective to support the new scientific practices.

This study is part of a doctoral research that has as its objective to provide semantic guidelines for structuring and publishing open notebook data, aiming at improvements in retrieving and sharing data.

7.2 OPEN NOTEBOOK SCIENCE

The term *Open Notebook Science* was coined by Jean-Claude Bradley in September 2006 to promote debates on open collaboration in science and developing more efficient research techniques. For Bradley (2010) the goal

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of open notebook science is making the details of experiments conducted in laboratories freely available on the Web, which does not restrict only successful.

For Schapira and Harding (2019) the opening and sharing of scientific research data recorded in notebook science are efficient and fast ways to disseminate data before it is published in peer-reviewed journals, and they present advantages in relation to the traditional way-release after publication.

First, by making data accessible in weeks, rather than keeping it hidden for years, it means that others will be able to take advantage of the research and avoid wasting redundant experimental time and resources. Second, open notebook science must include detailed protocols that can be reproduced, which is often not the case in peer-reviewed publications. Third, unsuccessful data, which are seldom released in the current publishing system but are provided in open notebook science, can therefore help to save time, resources, and knowledge (Schapira; Harding, 2019, p. 3).

According to Schapira and Harding (2019) the open notebook science includes several procedures performed during an experimental research in a way to ensure the successful replication of results. These sets of procedures are mentioned in the literature as research protocol, which is set as the main purpose of data dissemination and sharing, for it has a complete description of the procedures performed, the equipment adopted, and the reagents used during the research, besides declaring the intended purposes, the discussion of data found in the research, and it records the results achieved either partial or final. The protocols must be followed by textual documents and spreadsheets in case they are necessary for the interpretation of procedures for materialization of objects of study such as lines, dots, graphics, maps, spectra among others.

The proposal for opening research datasets recorded in notebook science is part of a bigger movement of Open Science called *e-Science*, characterized by the intensive use of technologies and collaborative efforts, which bring the opportunity of thinking about the new contexts and scientific practices. In this context, Foster (2018) classifies the notebook science as integral part of the third dimension *Open Reproducible Research*, of the open Science taxonomy, which constitutes in the act of offering to users free access to experimental elements to allow the reproduction of research regardless of its results.

7.3 FAIR PRINCIPLES

FAIR principles, an acronym for *Findable, Accessible, Interoperable* and *Reusable*, originated in 2014, during the international conference *Jointly designing a data FAIRPORT*, from a debate among representatives of several fields of knowledge, such as librarians, archivists, editors and research sponsors, members of *The Future of Research Communications and e-Scholarship* (FORCE11), to improve the research data ecosystem and work as guidelines to increase research data reuse in the context of *e-Science* (FORCE11, 2014).

This discussion resulted in four relevant principles, with guiding practices for data release that would be easily findable, accessible, interoperable, and reusable by machines and humans, in the face of the great amount of information generated by intensive contemporary Science in data. These principles incorporate characteristics that define that the resources, tools, vocabularies, and contemporary data infrastructure should be shown to help to find and reusing third-parties (FORCE11, 2014).

According to Wilkinson *et al.* (2016), the elements of FAIR principles are related, but are independent and separable and can be implemented in any combination, incrementally, as data providers evolve their structures to achieve a higher level of FAIR principles purpose. The authors clarified that these principles precede the choices of implementation, and they do not limit Technologies for implementation. Thus, this study associates FAIR principles to Web Semantic and *Linked Data*.

7.4 WEB SEMANTIC AND LINKED DATA

Web Semantic was started in 2001, by Tim Berners-Lee with the collaboration of Hendler and Lassila (2001), from the proposal of defining an efficient way to represent data on the Web and provide improvement in the quality of information retrieval, allowing, according to Santarém Segundo (2012, p. 106) “the users to obtain more accurate results and with information closer to what they really need”.

The term *Linked Data* is presented as principles for implementation of Web Semantic technologies to publish and promote the connection of data from different sources on the Web, in order to provide benefits to the data. These principles are: 1– use *Uniform Resource Identifier* (URIs) with names for things; 2–use URI HTTP, so people can look up these names; 3– when someone looks for a URI, provide useful information, using standards such as *Resource Description Framework* (RDF) and SPARQL; and 4– include *links* for other URIs so that the items related can be found. (Berners-Lee, 2006).

The consortium of World Wide Web (W3C) recommends a set of Technologies for releasing open data and connection with the Web, according to *Linked Data* principles. Among the Technologies, *Resource Description Framework* (RDF) and its serialization stand out, with RDF as a standard model adopted for the description of information structured on the Web, allowing machines to legibly represent information about a resource um (W3C, 2014).

W3C recommends a set of 35 (thirty-five) Best Practices (BP) for *Data on the Web Best Practices* (DWBP), to improve the coherence between provider and consumer, encourage and allow the continued expansion of the Web as a way for data exchange and promote reliable data reuse

The thirty-five BP to release data on the Web are distributed in categories and for each best practice a set of benefits is obtained, as presented in Table 1.

Table 1 – Best Practices and Benefits

Category	Best Practice	Benefits
Metadata	BP 1 – Provide metadata for human users and machines	Reuse, understanding, finding, and ability to process
	BP 2 - Provide descriptive metadata	Reuse, understanding and finding
	BP 3 - Provide structured metadata	Reuse, understanding, and ability to process

Category	Best Practice	Benefits
Licenses	BP 4 – Provide information on data license	Reuse and reliability
Data origin	BP 5 – Provide information on data origin	Reuse, understanding, and reliability
Data quality	BP 6 – Provide information on data quality and necessary adaptations	Reuse and reliability
Data version	BP 7 – Assign version for each dataset	Reuse and reliability
	BP 8 – Provide a history of versions	Reuse and reliability
Data identifiers	BP 9 - Use persistent URIs as datasets identifiers	Reuse, interconnection, finding, and interoperability
	BP 10 – Use persistent URIs as identifiers within datasets	Reuse, interconnection, finding, and interoperability
	BP 11 - Assign URIs to datasets versions	Reuse, finding, and reliability
Data formats	BP 12 – Use standardized data formats	Reuse and ease of processing
	BP 13 – Use neutral data representation to locations	Reuse and understanding
	BP 14 – Provide data in several formats	Reuse and processability
Data vocabulary	BP 15 – Reuse vocabularies, preferably standardized	Reuse, processability, understanding, reliability and interoperability
	BP 16 – Choose the correct level of formalization	Reuse, understanding, and interoperability

Category	Best Practice	Benefits
Data access	BP 17 – Allow complete mass access	Reuse and access
	BP 18 – Allow partial access to the datasets	Reuse, access, interconnection, and processability
	BP 19 - Provide data in several formats	Reuse and access
	BP 20 – Allow access in real time	Reuse and access
	BP 21 – Provide updated data	Reuse and access
	BP 22 – Explain the reasons when data is not available anymore	Reuse and reliability
	BP 23 – Provide data through API	Reuse, processability, interoperability, and access
	BP 24 – Use Web standard as APIs basis	Reuse, interconnection, interoperability, finding, access and processability
	BP 25 – Provide documents as far as API is added or changed	Reuse and reliability
	BP 26 – Avoid breaking changes in API	Reuse and interoperability
Data preservation	MP 27 – Preserve the identification and provide information on the field resource	Reuse and reliability
	MP 28 – Evaluate the coverage of a dataset before its preservation	Reuse and reliability
Feedback	MP 29 - Collect <i>feedback</i> from consumers	Reuse, understanding, and reliability
	MP 30 – Make the <i>feedback</i> publicly available	Reuse and reliability
Data enrichment	MP 31 – Enrich data, generating new data	Reuse, understanding, reliability and processability
	MP 32 – Offer complementary presentations	Reuse, understanding, access and reliability
Republication	MP 33 - Provide <i>feedback</i> to the original publisher	Reuse, interoperability, and reliability
	MP 34 – Follow the license terms	Reuse and reliability
	MP 35 – Cite original publication	Reuse, finding, and reliability

Source: Adapted from de Lóscio, Burle and Calegari (2017).

After presenting these BP, it is possible to analyze the semantic elements to describe the open notebook Science concerning data coverage being findable, accessible, interoperable, and reusable, from the application of FAIR principles, We Semantic Technologies and *Liked Data* concepts.

7.5 SEMANTIC ELEMENTS OF DESCRIPTION OF OPEN NOTEBOOK SCIENCE

It presents the result of metadata and vocabularies mapping that aim to describe and individualize the objects that compose the notebook Science ecosystem, especially regarding experimental research for structuring and publication of open notebook Science. The mapping presents a set of semantic elements, according to Table 2.

Table 2 - Mapping of metadata and vocabulary properties

Metadata Spreadsheet (Labels)	Vocabulary Property Schema.org, DC Terms, SKOS and RDA Element Sets
Identification of record	schema:identifier
Date and hour of record	schema:dateTime
Author ^	schema:author
• Date of birth	schema:birthDate
• Date of death	schema:deathDate
• Profession/Occupation	schema:hasOccupation
• Institution associated ^	schema:memberOf
• Department of Institution	schema:department
Contributor /Collaborator ^	schema:participant
• Date of birth	schema:birthDate
• Date of death	schema:deathDate
• Profession/Occupation	schema:hasOccupation
• Institution associated ^	schema:memberOf
• Department of Institution	schema:department
Institution ^	schema:sourceOrganization
Development Agency ^	schema:funder

Metadata Spreadsheet (Labels)	Vocabulary Property Schema.org, DC Terms, SKOS and RDA Element Sets
• Identification of the agent	schema:Identifier
• Controlled access point	skos:prefLabel
• Variable Access Point	skos:altLabel
• Field of activity	rdaa:P50387
• Language ^	schema:inLanguage
• Contact Information	schema:email
Title	schema:name
Subtitle	schema:alternativeHeadline
Language ^	schema:inLanguage
Format ^	dct:format
Type ^	dct:type
Total number of pages	schema:pagination
Spatial coverage ^	schema:location
Research period	schema:startTime
Audience	schema:audience
Intended purpose	schema:description
Results achieved	schema:result
Subject ^	schema:about
• Identification ^	schema:propertyID
• Controlled access point	skos:prefLabel
• Variable access point	skos:altLabel
• More extensive subject	skos:broader

Metadata Spreadsheet (Labels)	Vocabulary Property Schema.org, DC Terms, SKOS and RDA Element Sets
• More specific subject	skos:narrower
Description	schema:description
• Reagents ^	schema:activeIngredient
• InChIKey^	schema:identifier
• Equipments	schema:instrument
• Molecular formula^	schema:identifier
• Molecular weight^	schema:weight
• Measurement technique	schema:measurementTechnique
• Chemical names ^	skos:related
• Commercial name ^	skos:related
• Date of creation	schema:dateCreated
• Date of modification	schema:dateModified
• Closure research period	schema:endTime
• Status of the action	schema:actionStatus
• Error	schema:error
Data source	schema:provider
Declaration of provenance	dct:provenance
Use license	schema:license
Declaration of rights	dct:RightsStatement
Holder of rights	dct:rightsHolder
Size of the application	schema:fileSize
Necessary Software	schema:availableOnDevice

Metadata Spreadsheet (Labels)	Vocabulary Property Schema.org, DC Terms, SKOS and RDA Element Sets
Record of display	schema:RegisterAction
Control of use and user	schema:userInteractionalCount
Type of user interaction	schema:interactionType

Source: Silva (2020).

The first column presents the metadata identified through data modeling and insertion of attributes that describe the notebook Science specificities, plus elements that can be enriched with external vocabularies, such as a certain author's date of birth and date of death when it is the case. The elements marked with a triangle (◻) indicate the importance of reusing information from external *datasets* through URI whenever possible to avoid ambiguities, to ensure standardization and carry additional information to those required through metadata. The second column presents Schema.org, DC Terms, SKOS e RDA *Element Sets* vocabulary properties corresponding to metadata in the first column.

This structure presents an analysis of elements to be considered FAIR, considering that FAIR principles have been required by the academic Community, especially by development agencies, as evaluation criteria for funding research.

7.5.1 Analysis of semantic elements of notebook Science regarding being FAIR

The scope of the elements indicated in the development of guidelines for publishing notebook Science is discussed regarding data being findable, accessible, interoperable, and reusable from the application of FAIR principles, Web Semantic Technologies and *Linked Data* concepts, recommended by W3C.

7.5.1.1 Findable

The *findable* principle recommends four practices so that can be findable. The first principle, F1, indicates the assignment of identifiers globally exclusive and persistent, and the third principle, F3, indicates that data identifiers must be included. In this study, notebook Science were structured from the use of persistent indicators to describe names of objects, people, institutions, places and subjects, through the definition of metadata *tags*.

The recommendations of W3C highlight that the finding, use and citation of data on the Web depend fundamentally on the use of URIs in HTTP that can be checked on the internet. Thus, BP 9, 10 and indicate the use of persistent URI for the dataset and URI as identifier of datasets. In this regard, it is possible to observe the *tag* mapping directed to the use of identifiers or persistent URIs, such as people identifiers through vocabularies as ORCID and VIAF (*schema:author*, *schema:funder* and *schema:sourceOrganization*), indicators for spatial coverage using GeoNames (*schema:location*) vocabulary and subject indicators through LCSH, MeSH and PubChem vocabularies that can be presented from *schema:about* properties and its developments, as presented in Table 2.

In this perspective, the second principle *findable* (F2) recommends that a dataset should be described by metadata rich enough so that, once indexed in a Search mechanism, it can be found even without its persistent identifier. The BP 1, 2 and 3 recommend providing descriptive, structural and administrative metadata. The elements mapped describe data related to the experimental research, and it did not intend to be excessive but describe the information considered sufficient so that the researcher can analyze and choose data reproduction or repeatability.

In the occasion of implementing these guidelines, it is necessary to offer metadata for human Reading, Where W3C recommends providing metadata as part of a webpage HTML and as a separate text file. For machine interpretation, metadata can be provided in Turtle and JSON serialization format, or it can be incorporated in HTML page (HTML-RDFA or JSON-LD), and reuse existing standards and popular vocabularies. For notebook science, the integrated use of Schema.org and Dublin Core metadata standards were chosen to enable the detailed description of metadata values. Schema.org was selected to describe digital objectives regarding notebook science because it has numerous properties corresponding to experimental research, and Dublin Core because it has multiple properties to describe information such as provenance, format, and types of data. In addition to these, the SKOS vocabulary was adopted to refine metadata values.

The recommended practice in F4, the fourth principle *findable*, is that metadata is recorded and indexed in search mechanisms. The BP 12 collaborates with principle F4 when it recommends the use of standardized, machine-readable formats when releasing data on the Web. The indicated formats include, but are not limited to CSV, XML, HDF5, JDON e RDF serialization syntax such as RDF/XML, JSON or Turtle. BP 24 recommends adopting standards as the basis of APIs, and BP 35 suggests citing the original publisher as so it can be easily found. Those guidelines provided *tag schema:provider* to indicate the data source and to provide data reliability.

7.5.1.2 Accessible

According to Wilkinson *et al.* (2016) data accessibility is related to the use of standardized communication protocols, open and free, which offer authentication and access to metadata even when it is not available anymore.

W3C recommendation is enabling the access to the complete dataset of a certain research. In order to easily access these datasets, BP 17 recommends that the Web infrastructure must be implemented in a way to allow the mass access of a complete dataset with just a request, avoiding inconsistency in the individual data access over many retrievals, as well as allow the provision of data subsetting (BP18), in case consumers do not need the complete set.

The Web offers access using methods of hypertext transfer protocol (HTTP) for simple mass download of a file. Even if data is distributed in several URIs, it can be organized in a container model using the file transfer protocol to enable mass access to data. The distribution of data in several files allows the retrieval through an application programming interface (API), the most sophisticated retrieval method. BP 18, 20, 23 and 24 mention that an API is the most flexible approach for serving data subsets because they allow to personalize which data is transferred and provides data in real time.

The second principle *Accessible* (A2) suggests that metadata should be accessible, even when data is inaccessible, while W3C suggests, through BP 22, providing explanations for data that is not available, informing how it can be accessed and who can access it. In this regard, recommendations FAIR and BP can complement each other making data available, even when data is not available anymore, and still offer explanatory message.

7.5.1.3 *Interoperable*

The interoperability refers to the capacity of a system to easily communicate with others. For this purpose, it is necessary to adopt actions such as assign interconnected metadata and Web standards as the basis for APIs. In addition, in order to have a formal language, it is necessary to provide human and machine-readable metadata (BP 1 and 2), use persistent indicators (BP 9 and 10) and reuse standardized vocabularies (BP 15 and 16).

For structuring notebook science, vocabularies describing their purposes were selected, such as the description of authorities as refining attributes indicating dates, profession, field of activity, means of communication with the agents and the possibility of linking researchers to institutions and departments in to which they belong. In addition, vocabularies describing the specificities of an experimental research were sought such as names of chemical compounds, chemical properties, procedures carried out during the research, period of realization, status of the research and a way to inform if the research was successful; vocabularies enabling the description of data provenance were also sought. After detailing the attributes that describe the specificities of notebook science, Schema.org, DCTerms and SKOS vocabularies were chosen, in addition to value vocabularies such as GeoNames, VIAF, ORCID among others exemplified in F1 to F3. As a model of representation, the recommended practice is the use of RDF and its serializations, which is also mentioned in F2. Moreover, the use of widely recognized vocabularies enables the benefits of data interoperability, processability, understanding, reliability and reuse.

7.5.1.4 *Re-Usable*

This principle is especially important for the notebook science context because it reflects the application of the previous principles (findable, accessible and interoperable) to the structuring purpose that is data being reused by researchers in new research.

The principle R1 establishes that metadata must be described with plurality of accurate and relevant attributes, therefore, provenance, description of notebook Science specificities, administrative and use metadata were mapped. In order to describe textual values, the use of persistent identifiers is recommended with the purpose of data enrichment.

Principle R1.1, BP4 and BP34 highlight the importance of providing a type of license to avoid limitations in reusing and legally formalizing the provision of data to be reused in other works. Principle R1.2 and MP 5 recommend that metadata must be associated to its provenance. In these guidelines, the tags for data source (*schema:provider*) were mapped to indicate data provenance, provenance declaration (*dct:provenance*) to explain changes in the property and custody of an object, license (*schema:license*) to allow the object use, declaration of rights (*dct:RightsStatement*), holder of the rights (*dct:rightsHolder*) to indicate the name of the agent that has or manage the rights

of the object, date of creation (*schema:dateCreated*) and modification of data (*schema:dateModified*) to inform the original date and the modifications.

BP 13 suggests providing information on location parameter to avoid difficulties in understanding data that changes from one language to another, for example informing the language on the *tag schema:inLanguage* of the Schema.org standard.

BP 14 recommends, whenever possible, that data is available in multiple formats, when more than one match its intended use. When implementing these guidelines, it is recommended that data is converted to RDF/XML, JSON and Turtle formats, which meet BP 12 recommendations for using machine-readable format, BP 14 recommendation for multiple formats, BP 15 known and standardized vocabularies.

7.6 FINAL CONSIDERATIONS

The provision of administrative, descriptive, provenance, preservation and use metadata, with the indication of implementation from standardized, human-and-machine readable vocabularies, in addition to the recommendation for attribution of URIs for indicating names and data enrichment, can guarantee that notebook Science data are findable.

Following the recommendation for using APIs will enable data accessibility. In addition to these elements, it is recommended the use of contextual explanation on about data and its metadata in order to provide interoperability of data. It is noteworthy that unifying previous recommendations to the indication of a use license, preferably of public domain, as well as detailing metadata associated to data provenance, enables reusing notebook Science data released based on these guidelines. It is worth noting that not all recommendations related to accessibility principles are covered in these structuring guidelines; however, the recommendation remains for the occasion of implementation.

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